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Introduction to Monte Carlo Tools

*V. Lendermann*¹, *A. Nikitenko*², *E. Richter-Was*³, *P. Robbe*⁴, *M. H. Seymour*⁵

¹ Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany;

² Imperial College, London, UK; on leave from ITEP, Moscow, Russia;

³ Institute of Physics, JU/IFJ-PAN, 30-059 Krakow, ul. Reymonta 4, Poland;

⁴ Laboratoire de l'Accélérateur Linéaire, Université Paris-Sud, 91898 Orsay, France;

⁵ School of Physics & Astronomy, University of Manchester, UK, and Theoretical Physics Group, CERN.

Abstract

The activities of working group 5 ‘Monte Carlo Tools’ of the HERA–LHC Workshop are summarized. The group concerned itself with the developments and tunings of Monte Carlo models in light of the HERA–LHC connection, interfaces and libraries for parton density functions, Monte Carlo running, validation and tuning frameworks as well as some data analysis tools.

1 Introduction

The goals of working group 5 were

- to review existing and developing Monte Carlo (MC) models used for studies at HERA and the LHC;
- to examine and possibly improve MC models for the LHC physics using HERA data;
- to prioritize possible measurements at HERA which would allow tuning of these MC models;
- to pursue the development of frameworks for running, validating and tuning of MC and analysis programs;
- to improve and further develop common interfaces and libraries used with MC event generators;
- to review data analysis tools developed by the HERA collaborations which can be useful for studies at the LHC.

Both theorists and experimentalists from the HERA and LHC communities came together, in order to share their experience, identify crucial issues, and discuss the future developments of the programs, libraries and frameworks.

The physics topics discussed in the group have overlapped with those of all the other working groups in this workshop. Therefore many presentations were given in common sessions with other groups, most notably with working group 2 ‘Multijet Final States and Energy Flows’. These presentations covered the models of multiparton interactions, new developments in parton shower models, matrix element / parton shower (ME+PS) matching and simulations of multijet final states. The contributions to the present proceedings reviewing these studies are published in the chapter of working group 2. Further contributions are summarized below.

2 Libraries for Parton Density Functions

In the past, the PDFLIB library [1] was the standard package containing parametrizations of the proton, photon and pion parton density functions (PDFs). The LHC studies have necessitated the development of a new library which should include not only the central values of PDFs but also the error sets. The PDFLIB interface appeared not well suited to meet the new requirements. Therefore a new library, LHAPDF (Les Houches Accord PDF library [2]) was created following the Les Houches meeting in

2001. During this workshop the library was extensively developed by *M. Whalley* and *D. Bourilkov* [3]. Several recent PDF sets were included, both those by the leading theory groups and by the H1 and ZEUS collaborations. The fits are important for better estimations of PDF uncertainties. A particularly interesting cross check would be, for example, the comparison of the fits provided by the TeVatron collaborations with the independent predictions obtained by the DGLAP evolution of the HERA PDFs to the TeVatron region.

The photon and pion PDFs were also included in the library, thus allowing its use for all HEP analyses, in particular, for HERA studies. The library has thus developed to the level at which it can fully replace PDFLIB. Several tests of the applicability and performance of the library were made within the H1 collaboration (*V. Lendermann*).

Another topic discussed is the creation of a collection of diffractive PDF parametrizations. The project was presented by *F. P. Schilling* in a meeting of working group 4 ‘Diffraction’.

3 Monte Carlo event generators

The status and plans for major leading order (LO) and next-to-leading order (NLO) QCD programs, as well as generators with k_T factorisation were discussed.

3.1 Leading order Monte Carlo programs

Currently, the major FORTRAN MC event generators, PYTHIA [4] and HERWIG [5], are undergoing the transition to object-oriented software technologies. The C++ versions of both generators, PYTHIA7 [6] and HERWIG++ [7], are built in the common framework THEPEG [8] which is based on the CLHEP class library [9].

PYTHIA7/THEPEG includes some basic $2 \rightarrow 2$ matrix elements (ME), several built-in PDF parametrizations, remnant handling, initial- and final-state parton showers, Lund string fragmentation and particle decays. There have been plans to rework the fragmentation model, in order to include junction strings, and to implement multiple interactions (*L. Lönnblad*). However, *T. Sjöstrand* recently started a completely new C++ implementation, PYTHIA8 [10].

In parallel to the work on the C++ PYTHIA versions, the development of the FORTRAN PYTHIA6 continues. It remains the main platform for new physical concepts. Version 6.3 [11, 12] includes a completely new framework for simulation of parton showers and multiple interactions by *T. Sjöstrand* and *P. Skands*. Currently this version works for pp interactions only.

The development of HERWIG continues mainly in C++ (*S. Gieseke*, *A. Ribon*, *P. Richardson*, *M. H. Seymour*, *P. Stephens* and *B.R. Webber*). The current FORTRAN version 6.5 is foreseen as the final FORTRAN version of HERWIG (apart from possible bug fixes). It is interfaced to the JIMMY generator for multiple interactions (*J. M. Butterworth*, *J. R. Forshaw*, *M. H. Seymour*, and *R. Walker*).

HERWIG++ includes a new parton shower algorithm and an improved model of cluster fragmentation. The e^+e^- event generation is implemented in HERWIG++ 1.0. The next version including hadronic interactions is in progress. The plans for the near future are to fully implement the matrix element-parton shower matching according to the Catani-Krauss-Kuhn-Webber (CKKW) scheme [13], as well as multiple interactions. A new framework for accessing particle data and simulations of particle decays is currently being constructed by *P. Richardson*. The treatment of hadronic decays will include spin correlations.

Further physics models can be incorporated into the same THEPEG framework. In particular, it is planned to make a C++ version of ARIADNE [14] based on THEPEG (*L. Lönnblad*). ARIADNE implements the Dipole Cascade Model (DCM) [15, 16] as an alternative to the DGLAP-based shower models used in PYTHIA or HERWIG.

Despite the great success of ARIADNE in modelling hadronic final state observables, as measured at LEP and HERA, additional work is necessary to make ARIADNE fully suitable for modelling inter-

actions at the LHC. This was, in particular, shown in a study presented by Z. Czczyula on the impact of parton shower models on the generation of bbH , $H \rightarrow \tau\tau$ at the LHC [17]. The planned features include a remodelling of initial-state $g \rightarrow q\bar{q}$ splittings as well as the introduction of the $q \rightarrow g^*q$ process.

Another study was presented by N. Lavesson of ME+PS matching in ARIADNE on the example of W +jet production at the TeVatron [18]. It is also planned to include the matching to fixed order tree-level matrix elements *à la* CKKW [13, 18, 19] for the most common subprocesses at the LHC. When these plans are realised (we hope during 2006), it should be safe to use ARIADNE for LHC predictions.

An alternative C++ implementation is performed in the SHERPA program (T. Gleisberg, S. Höche, F. Krauss, A. Schälicke, S. Schumann, J. Winter) [20] which is capable of simulating lepton–lepton, lepton–photon, photon–photon and fully hadronic collisions, such as proton–proton reactions. In its current version SHERPA includes the ME generator AMEGIC++ providing the matrix elements for hard processes and decays in the SM, MSSM and the ADD model, the parton shower module APACIC++ containing virtuality-ordered initial- and final-state parton showers, ME+PS matching using the CKKW algorithm, the AMISIC++ module for a simple hard underlying event model taken from PYTHIA and an interface to the PYTHIA string fragmentation and hadron decays. Studies were presented on ME+PS matching considering W/Z +jet production at the TeVatron and at the LHC (S. Schumann) [18], and on the underlying event simulations (S. Höche) [12].

None of the above C++ programs is available for ep interactions yet, and so no applications and tests of these programs at HERA have been possible.

Further talks were given on the RAPGAP event generator [21] by H. Jung and on the ACERMC event generator [22] by B. Kersevan and E. Richter-Was. RAPGAP is one of the major generators used at HERA. It includes leading-order QCD matrix elements, LEPTO [23] and ARIADNE parton cascade models, as well as simulations of hard diffraction. Both ep and pp versions are available. Recently, the Les Houches Accord interface for fragmentation models was included; this allows the choice between the PYTHIA and HERWIG fragmentation models. This feature may allow better estimations of measurement uncertainties accounting for the transition from the parton to the hadron level of final states. It is planned to include double-diffractive scattering for pp collisions to allow simulation of diffractive Higgs production.

The ACERMC event generator simulates the Standard Model backgrounds to the Higgs production in pp collisions. It includes LO QCD matrix elements produced by MADGRAPH/HELAS [24], as well as both PYTHIA and HERWIG parton shower and fragmentation models via the Les Houches Accord interface. During this workshop, the ARIADNE parton shower model and the LHAPDF library were implemented. The program is also interfaced to TAUOLA [25] for precise treatment of τ decays and to PHOTOS [25, 26] for simulations of QED radiative decays. The study on the impact of parton shower models on generation of bbH , $H \rightarrow \tau\tau$ at the LHC [17], mentioned above, was performed using ACERMC.

The program can be linked with the ACERDET package [27] which provides a fast and simplified simulation of the expected ATLAS detector effects (energy smearing, acceptance corrections) as well as the usual analysis steps (jet reconstruction algorithms, isolation criteria, etc.). This allows a quick estimation of the feasibility of measurements in an LHC experiment, not necessarily by the members of the experimental collaboration.

3.2 NLO Monte Carlo programs

NLO QCD calculations are required to make theoretical predictions at the level of precision currently reached in particle scattering experiments. However, writing a hadron level MC program implementing an NLO model is a very complicated task, which has currently been solved only for a few pp reactions [28]. An important step forward would be an ep version of MC@NLO. It would be a major benefit for HERA studies of heavy quark and multijet production and would also allow an extensive validation of the NLO QCD calculations with HERA data. The development of the program started recently [29].

3.3 Monte Carlo programs with k_T factorization

The CASCADE event generator presented by *H. Jung* [30] provides an implementation of the CCFM model for parton cascades [31]. The program was very successful in describing hadronic final states at low x at HERA. First applications of CASCADE for the studies at the LHC were presented by *G. Davatz* [17]. The plans include an implementation of quark lines into CCFM cascades (currently, only gluon lines are implemented), as well as a new model for multiparton interactions based on the AGK cutting rules [32].

A reformulation of the CCFM model into the link dipole chain (LDC) model [33] provides a simplified formalism, which has been incorporated into the LDCMC program by *H. Kharraziha* and *L. Lönnblad* [14, 34]. An LDCMC version for deep inelastic ep scattering is available within the framework of the ARIADNE event generator. A pp version is planned.

In conjunction with these models, special sessions of working group 2 were dedicated to possibilities of determining the unintegrated parton distributions in the proton [35].

4 Comparisons of MC models with data

Models for particular subprocesses and their tuning using HERA data were reviewed in the corresponding working groups. As mentioned above, many discussions were carried out in the common sessions of working group 5 with the other groups.

One topic considered in WG5 is a comparison of leading proton data with several MC models (*G. Bruni, G. Iacobucci, L. Rinaldi, M. Ruspa*) [36]. The ep data from ZEUS and pp data from ISR and fixed-target experiments were confronted to the HERWIG (together with POMWIG [37] and SANG to simulate diffraction), LEPTO, ARIADNE and PYTHIA simulations. This exercise revealed that the simulation of the leading-proton momenta, both longitudinal and transverse to the beams, does not reproduce the properties of the data.

This study can be especially important for the understanding of diffractive processes and backgrounds for them at the LHC.

5 MC running, tuning and validation frameworks

During this workshop much progress was made in developing common frameworks that provide a convenient handling of MC and analytical programs and allow quick comparisons of MC simulations and analytical calculations with the results of HERA and other HEP experiments. The developments of HZTOOL/JETWEB, RUNMC and NLOLIB packages were presented and actively discussed.

The HZTOOL [38, 39] library provides a comprehensive collection of FORTRAN routines to produce various distributions using Monte Carlo event generators. The routines allow easy reproduction of the experimental distributions by modelling programs and give access to published data from the EMC, SPS, LEP, HERA and TeVatron experiments. A number of studies for the LHC and the future linear collider are also included. The library can be linked with all major FORTRAN MC event generators, and with a number of NLO QCD programs from the NLOLIB package (see below). The development of the library started within the workshop ‘Future Physics at HERA’ and steadily continued in the last few years.

In the current workshop, the emphasis was put on the HERA results relevant for the LHC [38]. Several measurements by H1 and ZEUS were implemented which allow tuning of multiparton interaction models in MC event generators (work by *D. Beneckenstein, A. Bunyatyan, J. M. Butterworth, H. Jung, S. Lausberg, K. Lohwasser, V. Lendermann, B. M. Waugh*). Common tunings of multiple interaction models based on the TeVatron and HERA results may constitute in the future an interesting outcome of the current efforts. Recent H1 and ZEUS results on heavy quark production in ep collisions were also added (*A. W. Jung, A. Geiser, O. Gutsche, P. Thompson*). In addition, calculations of benchmark cross-sections for heavy flavour production were included [40].

Based on HZTOOL, JETWEB [38,41] is a facility for tuning and validating Monte Carlo models through a World Wide Web interface. A relational database of reaction data and predictions from different models is accessed through a Java servlet, enabling a user to find out how well a given model agrees with a range of data and to request predictions using parameter sets that are not yet in the database.

The transition of experimental analysis frameworks and Monte Carlo generators to object-oriented software technologies necessitates a proper development of the MC running, tuning and validation frameworks. For this reason, HZTOOL/JETWEB is currently subject to a major redesign within the CEDAR ('Combined e-Science Data Analysis Resource for high energy physics') project [42]. CEDAR should comprise:

- an extensive archive of data from particle scattering experiments, based on the Durham HEP database [43];
- validation and tuning of Monte Carlo programs, parton distribution functions and other high-energy physics calculation programs, building on JETWEB;
- access to well-defined versions of these programs and code management support for developers;
- a standardized set of data formats for specifying HEP measurements as used in HepData and Monte Carlo event generator configurations as used in JETWEB;
- Grid compatibility for distribution of JETWEB Monte Carlo submissions and to enable secure addition of experimental data to the HepData catalogue by experimental collaborations.

A particularly important step in building CEDAR will be designing a C++ equivalent for HZTOOL, as well as providing an interface to the new C++ MC event generators.

A complementary approach using the object-oriented software design was realised in the RUNMC framework [44] by *S. Chekanov*. While JETWEB is a Web server system, RUNMC is a desktop application written in C++ and Java. It provides a unified approach to generate MC events and to analyse different MC models. All major FORTRAN MC event generators can be run via RUNMC. The output of FORTRAN MC programs is converted to C++ classes for further analysis and for graphical representation (histograms). The graphical user interface of RUNMC allows an initialization of MC models and histograms in a unified manner, and provides monitoring of the event generation. The program provides an interface to HZTOOL. It also allows loading of 'project files' which can contain external calculations, MC tunings, histogram definitions, etc. In particular, these files can include C++ data analysis code, similar to the HZTOOL FORTRAN analysis routines.

A further project, discussed in working group 5, is a common framework for the NLO QCD programs, NLOLIB [45], which was initiated within the workshop 'Monte Carlo Generators for HERA Physics'. Since hadron level Monte Carlo programs implementing QCD NLO calculations are not (yet) available for many processes, parton level NLO calculations are extensively used. NLOLIB is aimed at becoming a container for virtually all NLO QCD programs. It provides:

- a set-up for compiling and linking the programs on diverse UNIX platforms;
- a unified access to the NLO event records;
- a unified steering for parameters and settings;
- a unified access to PDF libraries;
- an interface to HZTOOL, thus allowing easy comparisons with experimental results;
- examples of the analysis code which can be linked with the library.

During the workshop the structure of the framework was further developed by *K. Rabbertz*. In addition to already implemented programs for ep (DISENT [46], DISASTER++ [47], MEPJET [48]) and e^+e^- (RACOONWW [49]) physics, an effort was made to integrate further ep programs: NLOJET++ [50] (*K. Rabbertz*) and JETVIP [51,52] (*T. Schörner-Sadenius*). The integration of the NLO programs for pp physics is surely possible, but requires additional effort.

6 Data analysis tools

Apart from MC related topics, general analysis tools, aimed at searches for specific final states, were presented.

One such tool is SBUMPS [53], currently being developed by *S. Chekanov*, which performs automatic searches for resonance peaks in invariant-mass distributions of two or more tracks. The program can be useful for searches of new states as well as for the reconstruction of known resonances.

Recently, interest in hadron spectroscopy at HERA increased sharply with the observations of narrow peaks in inclusive invariant-mass distributions which can be interpreted as pentaquarks [54]. These studies have inspired the development of the automated peak searching tool, which can be used in data analyses at any particle scattering experiment.

A general strategy for searches for new physics was presented by *S. Caron*. The approach was developed and used by the H1 Collaboration for searches of new phenomena at HERA [55]. It involves a statistical algorithm to search for deviations from the Standard Model in the distributions of the scalar sum of transverse momenta or invariant mass of final-state particles and to quantify their significance.

7 Conclusions

A number of interesting developments of MC models, programs, libraries and frameworks were presented in working group 5. The general status and prospects for major established and currently developed MC generators were reviewed. In common sessions with working group 2, the models of multiparton interactions, new developments in parton shower models, matrix element/parton shower matching and simulations of multijet final states were extensively discussed. Direct communication between theoreticians and experimentalists from the HERA and LHC communities allowed the pursuit of several developments and studies. In particular the recent advances in the development of the LHAPDF library, HZTOOL, RUNMC and NLOLIB frameworks were inspired by discussions within working group 5. It is hoped that this will help further studies on validation and tuning of the MC models for multiparton interactions, parton showers, and heavy flavour production.

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